EXPERIMENT No. 1

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Spectral Identification No : 1

A] Preliminary Observation

I] IR Spectroscopy

Observation	Inference
a) Strong observation at 1724 cm^{-1}	C=O stretching i.e. acid, ketone, aldehyde may be present
b) Medium observation in region 3100 - 2900 cm^{-1}	C-H stretching aryl/vinyl (sp^2) & alkyl C-H (sp^3) may be present

II] ^1H NMR Spectroscopy

Observation	Inference
a) Total 4 peaks are present	4 types of proton present in the structure.
b) 2 peaks are present in the region 6.5 - 8.5 ppm	Aromatic ring is present

III] ^{13}C NMR Spectroscopy

Observation	Inference
a) Total 7 peaks are present	7 types of carbon atom is present.
b) 4 peaks are present in region 100 - 170 ppm	Aromatic ring is present

IV] UV Spectroscopy

Observation	Inference
a) There are 2 peaks in UV spectrum about 220nm	Compound is conjugate

Teacher's Sign

II] ^1H NMR spectrum

Observation	Inference
a) Total 4 peaks are present	Total 4 type of proton present
b) 2 peaks at 6.5 - 8.5 ppm	Aromatic ring present
c) There are 2 doublets in aromatic region.	Para - disubstituted aromatic ring present.
d) Singlet peak at 3.9 ppm	Due to CH_3 adjacent to O
e) Singlet peak at 2.5 ppm	Due to CH_3 at aromatic.

III] ^{13}C NMR spectrum

Observation	Inference
a) Total 7 peaks are present	7 type of carbon is present
b) 4 peaks are present in region 100 - 170 ppm	Aromatic ring is present
c) Signal at 169 ppm	Due to ester carbon atom
d) There are 4 peaks in aromatic region i.e. 100 - 170 ppm	Para disubstituted benzene ring present
e) Out of 4 aromatic signal, 2 are missing in DEPT 135	2 quaternary C-atom present in aromatic ring.
f) Signal at 79 ppm in proton decoupled spectrum.	Due to solvent
g) Signal at 52 ppm in DEPT 135	Due to CH_3 adjacent to O
h) Signal at 22 ppm in DEPT 135	Due to CH_3 at aromatic

IV] UV Spectrum

Observation	Inference
a) 2 peak in UV at 220 nm	Compound is conjugate
b) λ_{max} 238 nm ($\log_{10} \varepsilon$ 4.2)	Due to $\pi \rightarrow \pi^*$ transition
c) λ_{max} 281 nm ($\log_{10} \varepsilon$ 2.7)	Due to $n \rightarrow \pi^*$ transition

Teacher's Sign :

V] Mass Spectrum

Observation	Inference
a) Molecular ion peak $M^{+\cdot}$	m/e = 150
b) Base peak	m/e = 119

B] Determination of molecular formula

Rule of 13 : $\frac{M}{13} = n + r$

No. of carbon = $\frac{M}{13} = \frac{150}{13} = 11$

No. of hydrogen = $M - (C \times 12) = 150 - (11 \times 12)$
$= 150 - 132 = 18$

∴ Base formula : $C_n H_{n+r} = C_{11}H_{11+7} = C_{11}H_{18}$

Molecular formula	Add element	Reason of adding	Substract equivalent	Modified formula	IHD
$C_{11}H_{18}$	-	-	-	$C_{11}H_{12}$	3
$C_{11}H_{18}$	O	Carbonyl group	CH_4	$C_{10}H_{14}O$	4
$C_{10}H_{14}O$	O	IHD is insufficient	CH_4	$C_9H_{10}O_2$	5

∴ Molecular formula is $C_9H_{10}O_2$

C] Detail Observation

I] IR spectrum

Observation	Inference
a) Strong observation at 1724 cm^{-1}	C=O stretching i.e. carbonyl group is present.
b) Medium observation at region 3100 - 2900 cm^{-1}	C-H stretching alkyl (sp^3) present.
c) Peak at 1600 - 1610 cm^{-1}	C=C stretching, aromatic ring is present.
d) Strong observation near 1100 - 1300 cm^{-1}	C-O stretching is present

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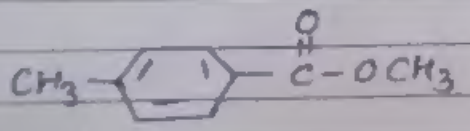
• Result:
The structure for given spectral data is



Teacher's Sign

EXPERIMENT: No.

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- Spectral identification No :- 2

A] preliminary observation

I] IR spectroscopy :-

	Observation	Inference
a)	Strong observation at 1718 cm^{-1}	carbonyl group present
b)	Medium observation at 3000 cm^{-1}	Alcohol group may be present.

II] ^1H NMR Spectroscopy

	Observation	Inference
a)	Total 3 peaks are observed	3 types of protons are present.
b)	There is no peak region to 6.5 - 8.5 ppm	This is an aliphatic compound.

III] ^{13}C NMR spectroscopy

	Observation	Inference
a)	Total 4 peaks are observed	4 types of carbon are present.
b)	Peak at 210 ppm	carbonyl carbon is present

IV] UV spectroscopy :-

	observation	Inference
a)	peak at 265 nm	So compound is conjugated.

V] Mass spectrum

	observation	Inference
a)	Molecular ion peak $M^{+\cdot}$	m/e = 72
b)	Base peak	m/e = 43

Teacher's Sign. :

B) Determination of Molecular formula :-

* Rule of 13 : $\frac{M}{13} = n+r$

No. of carbon $\frac{M}{13} = \frac{72}{13} = 5$

No. of Hydrogen $M - (C \times 12)$
$= 72 - (5 \times 12)$
$= 72 - 60$
$= 12$

∴ Base formula = $C_nH_{n+r} = C_5H_{12}$

Molecular formula	Add Element	Reagent of Adding	Substract equivalent	Modified molecular formula	IHD
C_5H_{12}	-	-	-	C_5H_{12}	$x + \frac{y}{2} - \frac{z}{2}$ $5 + 1 - \frac{12}{2}$ $6 - 6$ $= 0$
C_5H_{12}	O	Carbonyl group	CH_4	C_4H_8O	$x+1 - \frac{y}{2}$ $4+1 - \frac{8}{2}$ $5 - 4$ $= 1$

∴ Molecular formula : C_4H_8O

C] Detail observation :-

I] IR Spectrum -

Observation	Inference
a) Strong observation at 1718 cm^{-1}	carbonyl group aldehyde, ketone may be present.
b) medium observation at 3000 cm^{-1}	C-H stretching alkyl (sp^3) present
c) Peak at 1100 - 1200 cm^{-1}	C-O stretching ester or acid, ketone or aldehyde may be present

II] ^1H NMR Spectrum :

Observation	Inference
a) Total 3 peaks are observed	3 type of hydrogen are present
b) There is no peak region between 8.5 to 9.5 ppm	This is not aldehydic group is not present.
c) peak at 2.4 ppm shows quadret	so CH_3 is adjacent to CH_2
d) peak at 2 ppm shows singlet	so CH_3 is adjacent to carbonyl carbon
e) Triplet peak at 0.8 ppm	so CH_3 is adjacent to CH_2

III] ^{13}C NMR Spectrum

observation	Inference
a) total 4 peaks are observed	4 type of carbon is present
b) peak at 216 ppm	carbonyl carbon present
c) peak at region 30-50 ppm	due to CH_2 group
d) peak at region 20-30 ppm	due to $-CH_3$ group
e) peak at region 0-10 ppm	due to $-CH_3$ group
f) Singrial at 99 ppm in proton decoupled spectrum	due to solvent

IV] UV Spectrum -

a) Peak at 265 nm	so compound is conjugate because $\pi \to \pi^*$ transition

V] Mass Spectrum -

a) molecular ion peak M^+	m/e =
b) Base peak	m/e =

1] mass spectrum :-

Observation	Inference
a) molecular ion peak m^+	m/e = 192
b) Base peak	m/e = 135

- Determination of molecular formula :-
- Rule of 13 :- $\frac{m}{13} = n+r$

no. of carbon = $\frac{M}{13} = \frac{192}{13} = 16$

no. of hydrogen = $m - (C \times 12) = 192 - (16 \times 12)$
$= 192 - 162$
$= 24$

∴ Base formula = $C_nH_{n+r} = C_{16}H_{16+10} = C_{16}H_{26}O_4$

molecular formula	Add Element	Reagent of adding	substract equivalent	modified molecular formula	IHD
C_nH_{2n}	-	-	-	$C_{16}H_{24}$	$n+1 = y/2$ $= 16+1 = 24/2$ $= 16-12$ $= 3$
$C_{16}H_{24}$	O	carbonyl group	CH_4	$C_{15}H_{20}O$	4
$C_{15}H_{20}O$	O	IHD is insufficient	CH_4	$C_{12}H_{16}O_2$	5

∴ Molecular formula = $C_{12}H_{16}O_2$

- Detail observation :-

II] IR spectrum :-

observation	Inference
a) Peak at 1765 cm^{-1}	c=o stretching carbonyl grp present
b) Strong observation at 3000 cm^{-1}	c-H stretching alkyl (sp3) present
c) Peak at 1600 - 1500 cm^{-1}	c=c stretching, benzene present
d) Peak at 1200 - 1300 cm^{-1}	c-o stretching, ether, ester acid present.
e) Peak at 820 cm^{-1}	c-H stretching para substituted.

I] ^{1}H NMR spectrum :-

observation	Inference
a) there are 6 peaks observed	6 type of hydrogen present
b) 2 peaks present at 6.8-7.5 ppm	aromatic ring is present
c) signal at region 6-7.5 ppm	6.8 - 7.5 is due to aromatic ring
d) signal at region 1-1.5 ppm	1.2 - 1.4 is present.
e) there are doublet in region 6.5 - 7.5 ppm	as it is para disubstituted and aromatic ring present

III] ^{13}C NMR spectrum

observation	Inference
a) there are 8 peaks present	8 type of carbons present
b) peak at 115-160 ppm	aromatic ring is present
c) peak at range 160-180 ppm.	c-o stretching acid, ester, amide is present.
d) peak at region 50-60 ppm	there c-o present due to solvent
e) peak at 77 ppm	c=c stretching alkene present
f) peaks at 150 ppm	c-o stretching acid, ester, amide is present
g) peak at region 20-30 ppm	

IV] UV spectrum :-

observation	Inference
a) a peak at about 260-290 nm	compound is conjugated
b) peak at λ_{max} 262 nm ($\log\varepsilon$ 2.6)	due to $\pi \to \pi^*$ transition
c)	

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Spectral identification No - 3

A] preliminary observation -

I] IR - Spectroscopy -

	Observation	Inference
a)	strong observation at 1766 cm^{-1}	C=O stretching carbonyl group is present.
b)	strong observation at 3000 cm^{-1}	C-H stretching alkyl (sp^3) present.

II] ^1H NMR Spectroscopy

	Observation	Inference
a)	There are 4 peaks are observed	Total 4 type of proton are present.
b)	2 peaks present at region 6.5 - 8.5 ppm.	Aromatic ring may be present

III] ^{13}C NMR Spectroscopy

	Observation	Inference
a)	There are 8 peaks are observed	Total 8 type of carbon are present.
b)	peak at range 110 - 160 ppm.	Aromatic ring may be present.

IV] UV spectrum :-

	Observation	Inference
a)	peak at 262 nm & 269 nm	Compound may be conjugated.

Teacher's Sign

Sundaram

• structure :- $H_3C-CH_2-\overset{O}{\overset{\|}{C}}-CH_3$

• mass fragmentation :-

$H_3C-\overset{O}{\overset{\|}{C}}-CH_2-CH_3 \xrightarrow{e^-} \left[CH_3-\overset{O}{\overset{\|}{C}}-CH_2-CH_3\right]^{+\cdot} \xrightarrow{-CH_2=CH_2}$

$\left[CH_3-\overset{O}{\overset{\|}{C}}\right]^{+}$
m/e = 43

$\xrightarrow{-CH_3^{\cdot}}$ $\left[CH_3-CH_2\right]^{+}$
m/e = 29

$\xrightarrow{-CO}$ $\left[CH_3-\overset{}{C}-CH_2\right]^{+}$
m/e = 57

Thus:
From above spectral evidence, following structure can be confirmed:

$$CH_3-\overset{O}{\overset{\|}{C}}-CH_2-CH_3$$

• Results :-
The structure for given spectral data is

$$CH_3-\overset{O}{\overset{\|}{C}}-CH_2-CH_3$$

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Spectral identification No:- 9

A] Preliminary observation

I] IR Spectroscopy

	Observation	Inference
a)	strong observation at 1690 cm^{-1}	C=O carbonyl group is present.
b)	medium observation at 1300 - 1200 cm^{-1}	C-O stretching alcohol, ether may be present.

II] ^{1}H NMR Spectroscopy -

	Observation	Inference
a)	Total 3 peaks are present.	3 type of proton is present.
b)	Signal at region 7-8 ppm.	Aromatic ring may be present.

III] ^{13}C NMR Spectroscopy -

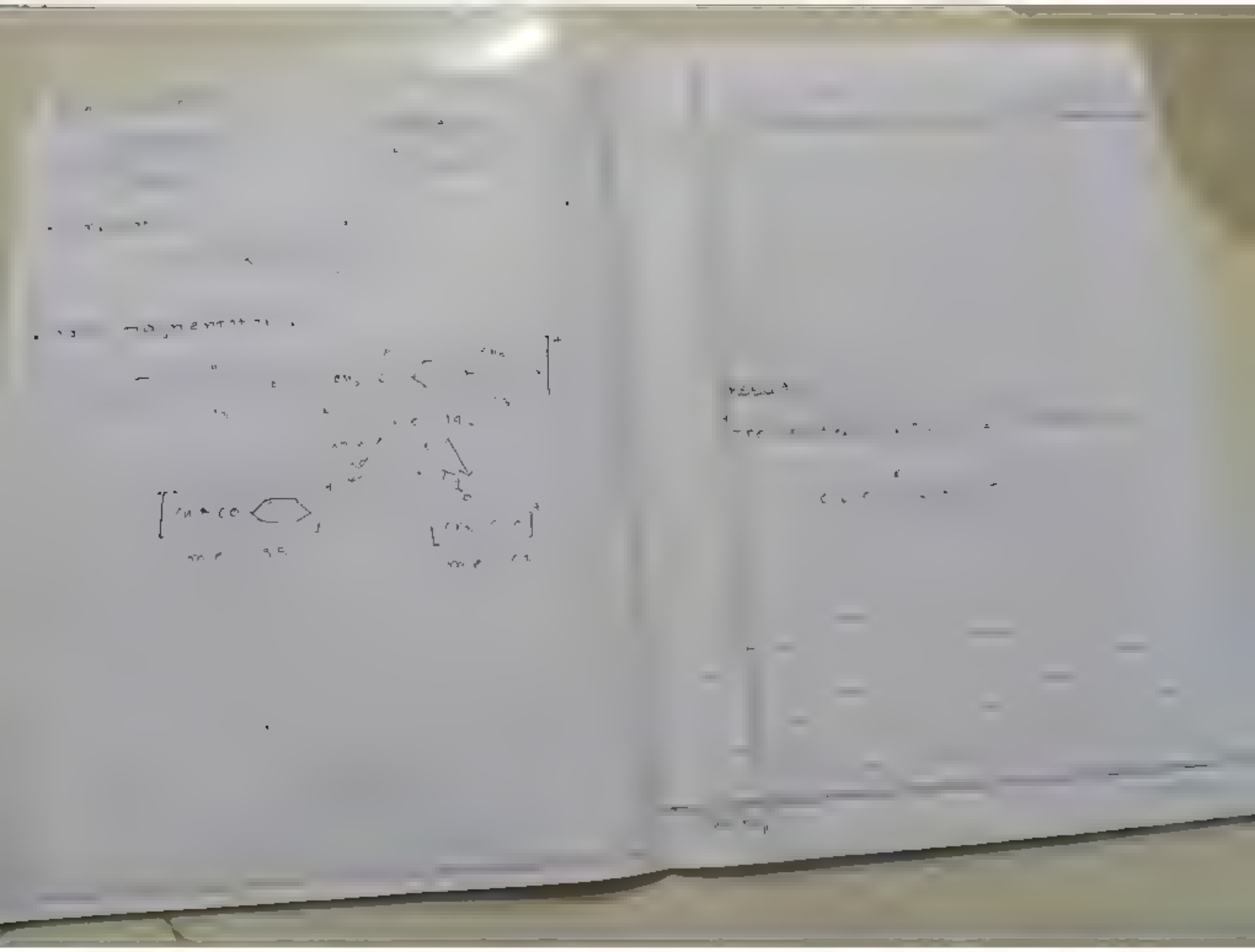
	observation	Inference
a)	Total 6 peaks are present.	6 type of carbon is present.
b)	4 peaks are present at region 120-160.	Aromatic ring may be present.

IV] UV Spectrum :-

	observation	Inference
a)	peaks at 255 nm	compound may be conjugated.

Teacher's Sign.:

Sundaram



Determination of molecular formula

Mole. formula	Add element	Reason of adding	Substraction eq. element	Modified molecular formula	IHD
[illegible]	C	Carbonyl group	CH4	[illegible]	2
[illegible]	C	Present in mass frag.	[illegible]	[illegible]	5

Molecular formula [illegible]

- Detail observation -

I) IR spectrum

Observation	Inference
a. strong observation at 1690 cm⁻¹	C=O carbonyl group is present
b. medium observation at 3000 – 3500 cm⁻¹	C–O stretching alcohol, ether may be present
c. peak at [illegible] cm⁻¹	C–C stretching benzene present
d. Peak at [illegible] cm⁻¹	para substituted C–H stretching

II) [illegible] spectroscopy

Observation	Inference
[illegible]	[illegible]

III) ¹³C NMR spectroscopy

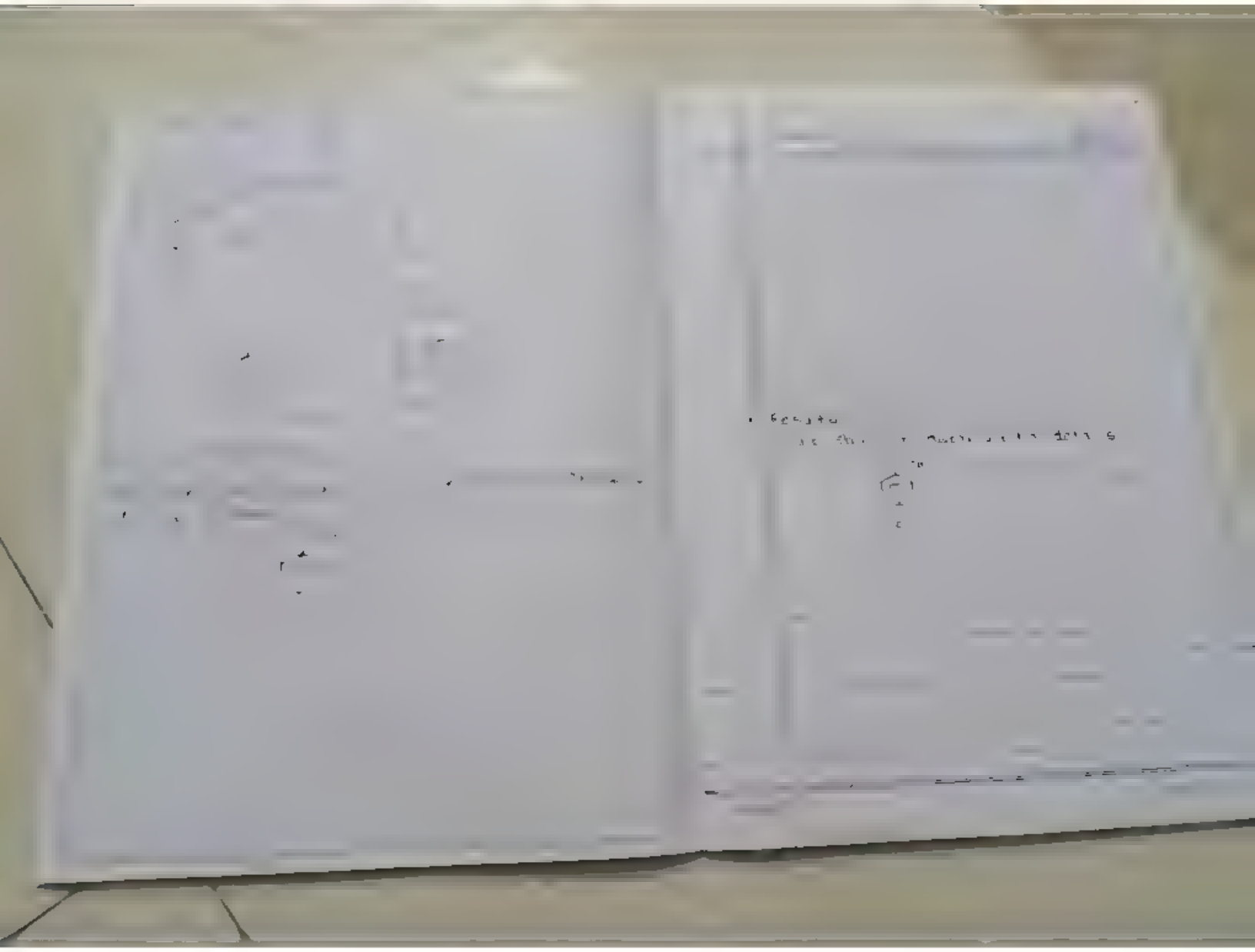
Observation	Inference
a. [illegible]	[illegible]
b. [illegible]	[illegible]
c. [illegible]	[illegible]

IV) [illegible] spectrum

Observation	Inference
a. peak at [illegible]	[illegible]
b. [illegible]	[illegible]

V) Mass spectrum

Observation	Inference
a) [illegible]	[illegible]
b) Base peak [illegible]	[illegible]



13

Date

Spectral identification No-5

A] Preliminary observation -

I] IR Spectroscopy -

observation	Inference
a) strong observation at 1743 cm^{-1}	Carbonyl C=O stretching
b) Strong observation at 1738 cm^{-1}	Carbonyl C=O stretching carboxylic acid, ester present

II] ^1H NMR spectroscopy -

observation	Inference
a) Total 3 peaks are present	3 type of proton present
b) peak at region 7.8 ppm	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy -

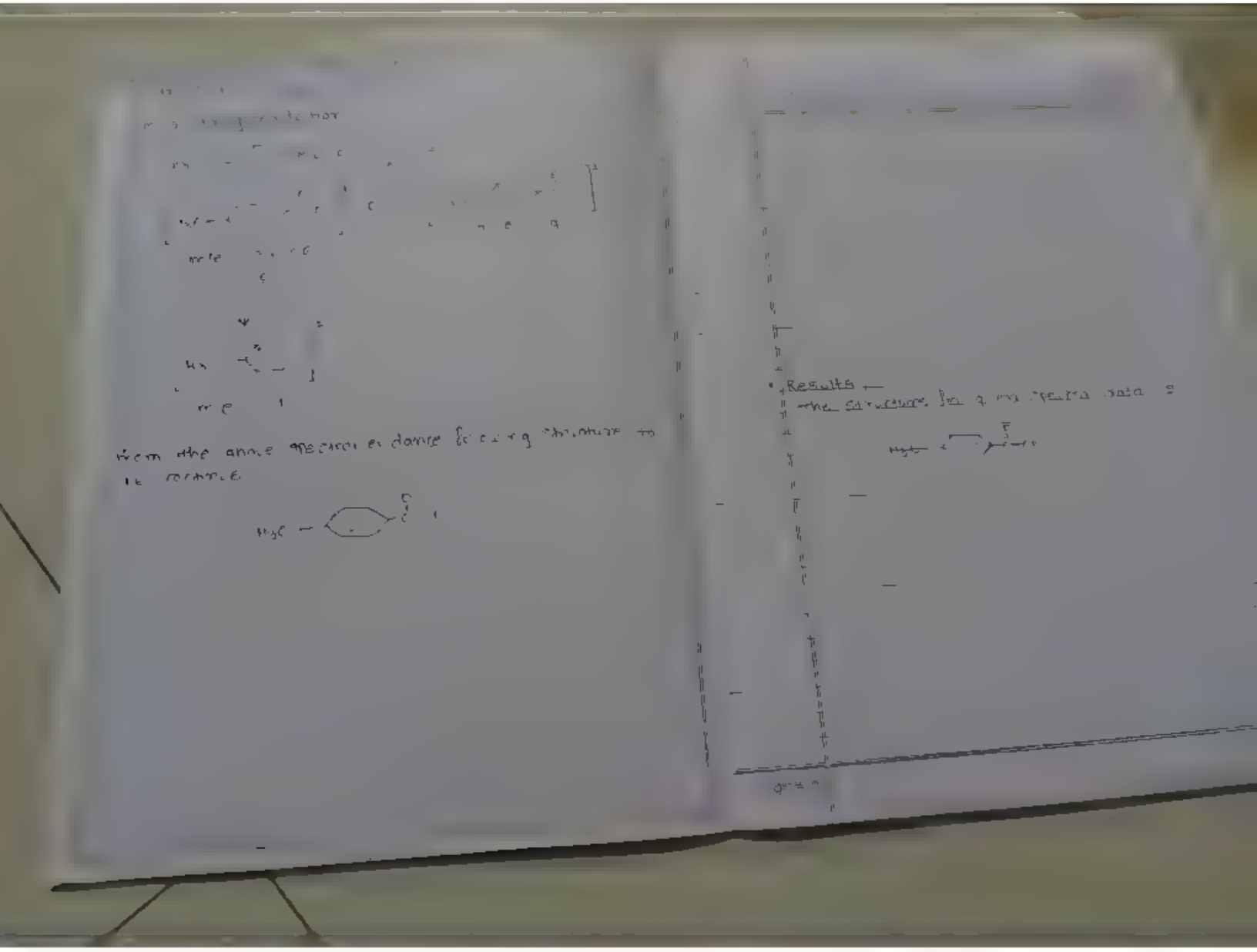
observation	Inference
a) Total 6 peaks are present	Total 6 type of carbon present
b) peak at region 160-180 ppm:	Carbonyl C=O stretching acid ester, amide present.

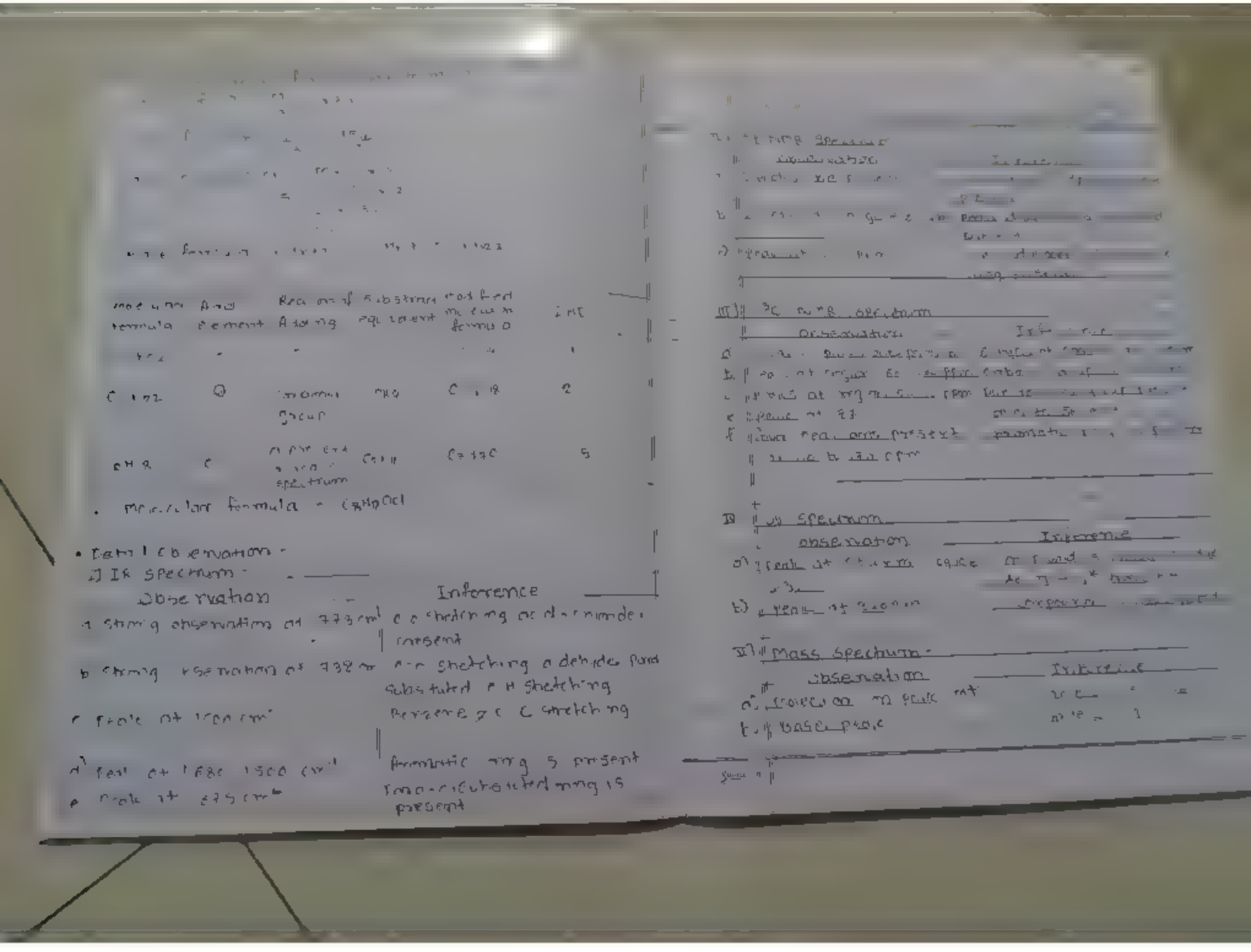
IV) UV spectrum -

observation	Inference
a) peak at about 220 nm	So compound may be conjugated

V] Mass spectrum -

observation	Inference
a) Molecular peak ion $M^{+\cdot}$	m/e = 154, 156
b) Base peak	m/e = 119




Observation
Inference

Spectral identification No - 6

Preliminary observation -

I] IR Spectroscopy -

observation	Inference
a) Observation at 1673 cm^{-1}	c=o stretching aldehyde, ketone may be present
b) Observation at 1600 cm^{-1}	c=c stretching benzene may be present

II] ^{1}H NMR Spectroscopy -

observation	Inference
a) 3 peaks are observed	Total 3 peaks types of proton are present
b) Two peaks present in region 7-8 ppm.	Aromatic ring may be present.

III] ^{13}C NMR Spectroscopy -

observation	Inference
a) Total 6 peaks are observed.	Total 6 types of carbon are present.
b) Peak present at region 110-160 ppm.	Aromatic ring may be present.

IV] UV Spectrum -

observation	Inference
a) Peak at above 220 nm	compound may be conjugated.

Inference

- Spectral identification No - 7
- Preliminary observation -

I] IR spectroscopy -

	Observation	Inference
a)	Strong peak at region 1720 cm^{-1}	C=O stretching ketone & aldehyde may be present.
b)	medium peak at region 3000 - 2700 cm^{-1}	C-H stretching alkane may be present.

II] ^{1}H NMR Spectroscopy -

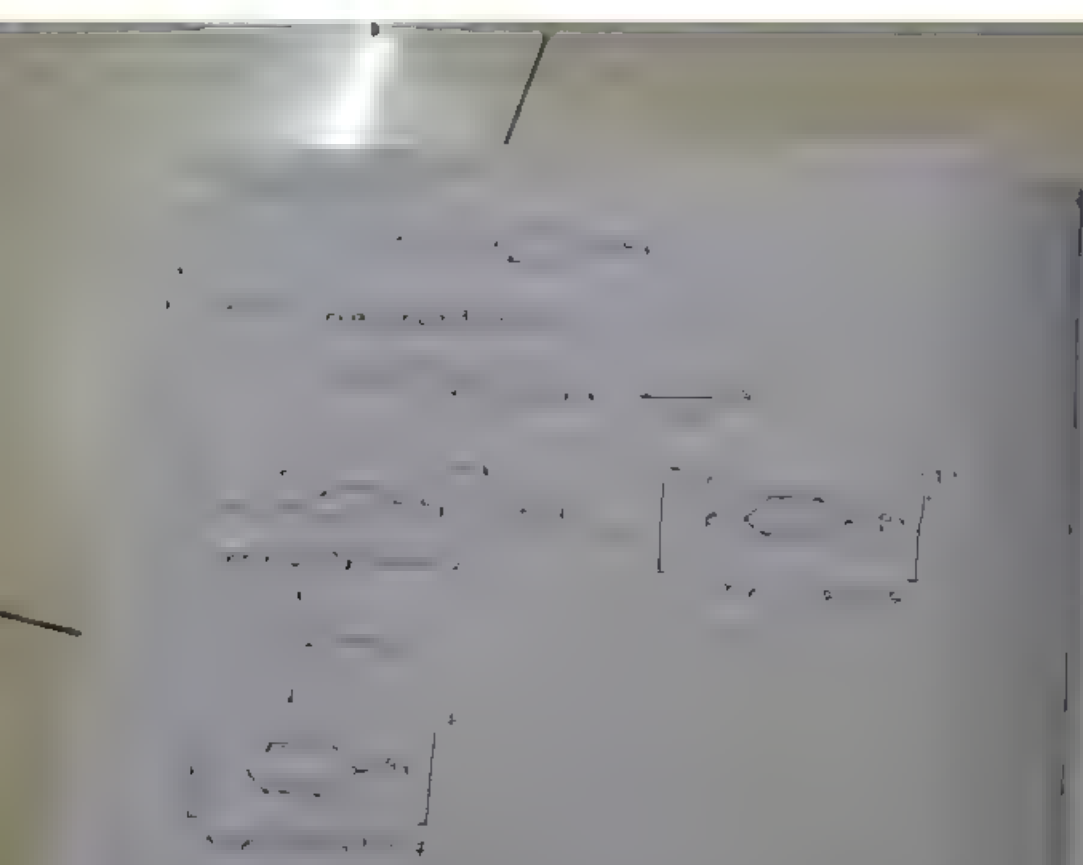
	Observation	Inference
a)	there are 4 peaks are observed	Total four type of proton are present
b)	Two peaks at region 6.5 - 8.5 δ ppm	Aromatic ring may be present.

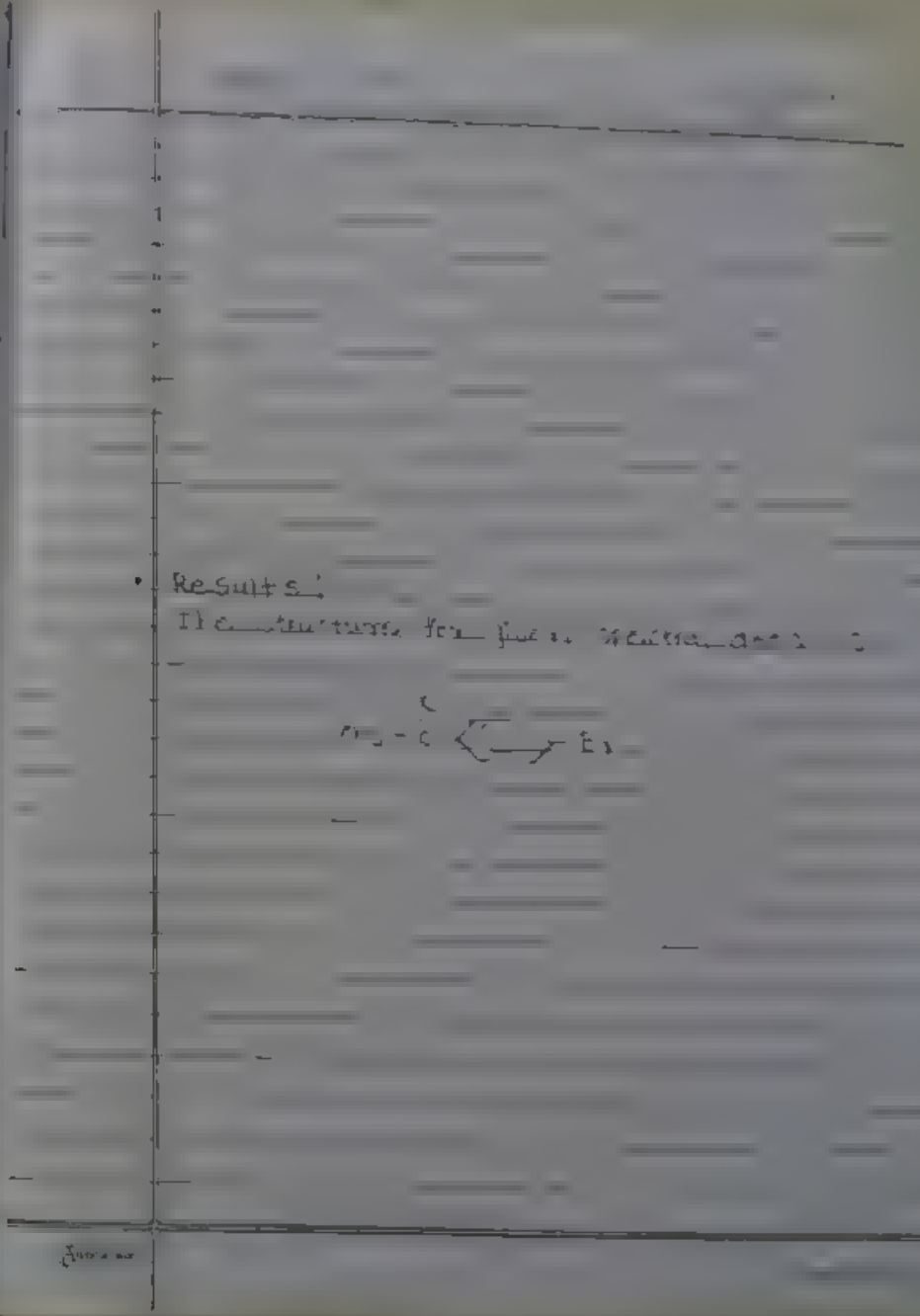
III] ^{13}C NMR spectroscopy -

	Observation	Inference
a)	There are 6 peaks are observed.	Total 6 type of carbon are present
b)	peak observe at 160 - 190 ppm.	carbonyl group may be present.

IV] UV spectrum -

	observation	Inference
a)	peak at above 220 nm	compound may be conjugated

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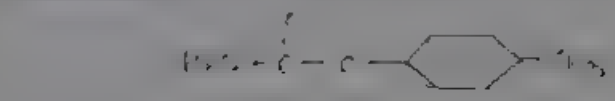
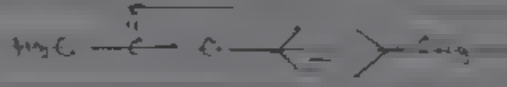


Results :-

The formula for given structure is



molecular formula	reason of unsaturation	equivalent molecular formula	IHD
[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	compound	[illegible]	[illegible]
[illegible]	insufficient	[illegible]	5

- Detail observation
- 1 IR spectrum

Observation	Inference
[illegible] strong peak at [illegible]	C=C stretching ketone aldehyde present
[illegible] peak at [illegible]	C-H stretching alkane present
[illegible]	C=C stretching [illegible] ketone present

II) ^1H NMR spectroscopy

Observation	Inference
[illegible]	[illegible]
[illegible]	[illegible]

III) ^{13}C NMR spectroscopy

Observation	Inference
a) [illegible]	[illegible]
b) peaks at [illegible] ppm	[illegible] present
c) Doublet peak at [illegible] ppm	[illegible]

IV) UV Spectrum

Observation	Inference
a) peak at [illegible] nm	[illegible]
b) peak at above [illegible]	compound is [illegible]

V) Mass spectrum

Observation	Inference
a) molecular ion peak M^+	m/e = [illegible]
b) Base peak	m/e = [illegible]

Spectral identification no 8

A) Preliminary observation -

I] IR spectroscopy

observation	Inference
a) Strong peak at 3322 cm^{-1}	O-H stretching may be present
b) Peak at 1085 cm^{-1}	C-O stretching may be present

II] $^1H^*$ NMR spectroscopy -

observation	Inference
a) They are five peak are observed	Total 6 peaks are type of proton.
b) peak at region 6.5 - 8.5 ppm	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy -

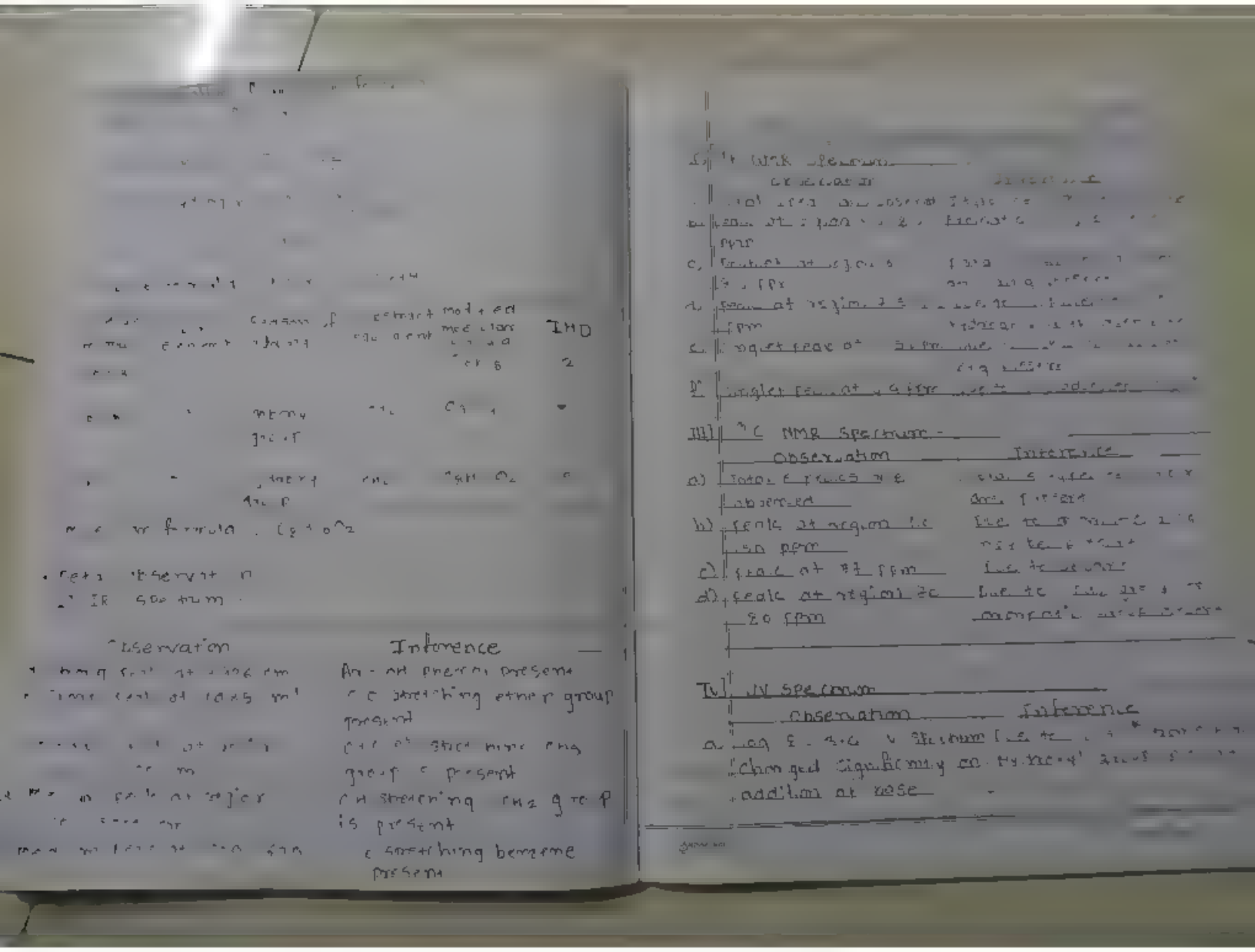
observation	Inference
a) There are 6 peaks are observed	Total 6 type of carbon are present.
b) Peak at 110 160 ppm	Aromatic ring may be present

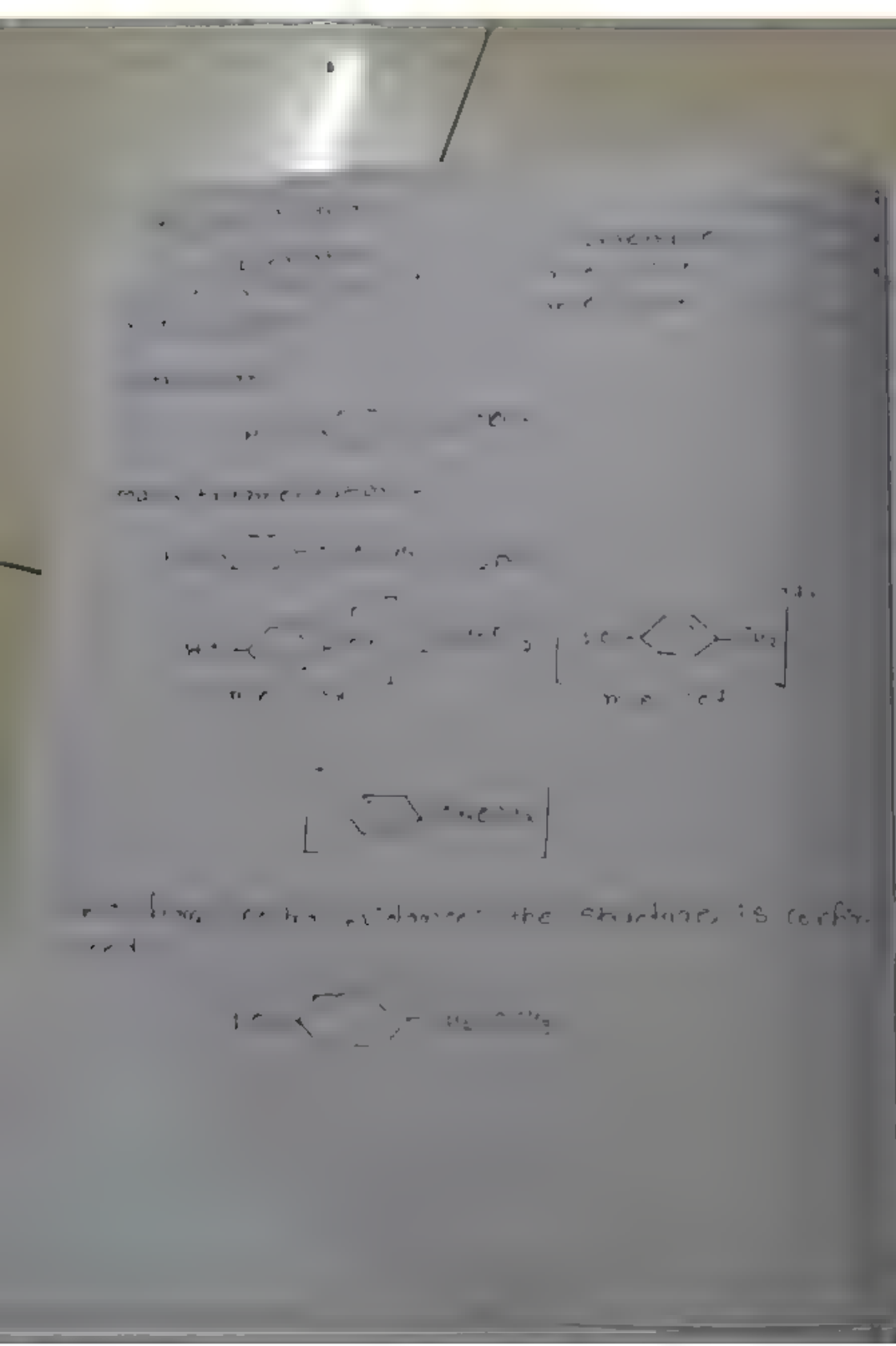
IV] UV spectrum -

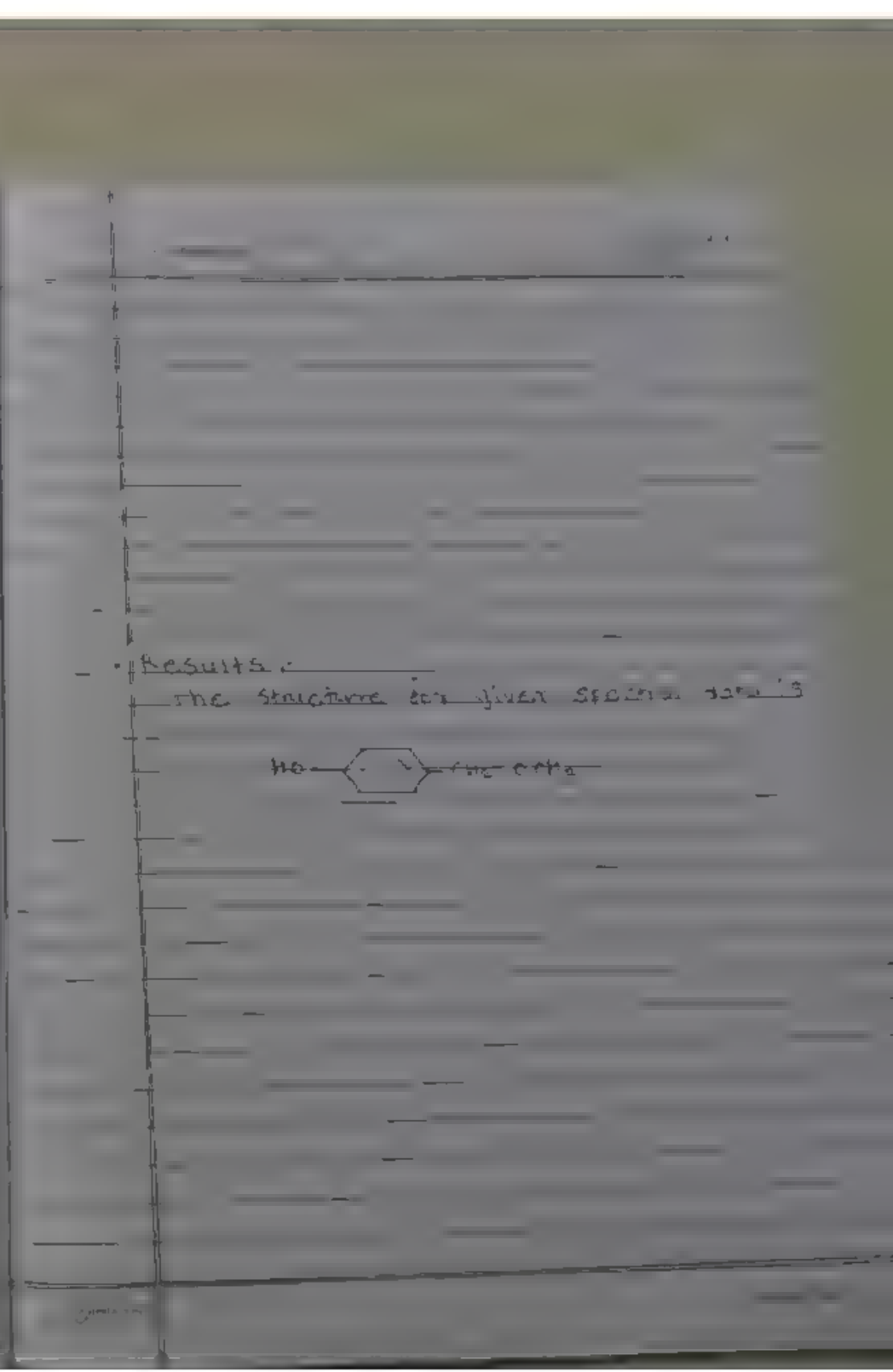
observation	Inference
a) log ε - 3.6 U.V spectrum	due to $\pi \rightarrow \pi^*$ transition hydroxy group present

V] Mass spectrum -

observation	Inference
a) Molecular peak ion M^+	m/e = 138
b) Base peak	m/e = 107







Results:

The structure for given spectral data is

EXPERIMENT [No]

observation	Inference
a) [illegible]	[illegible]
b) [illegible]	[illegible]

I. ^{1}H NMR Spectroscopy -

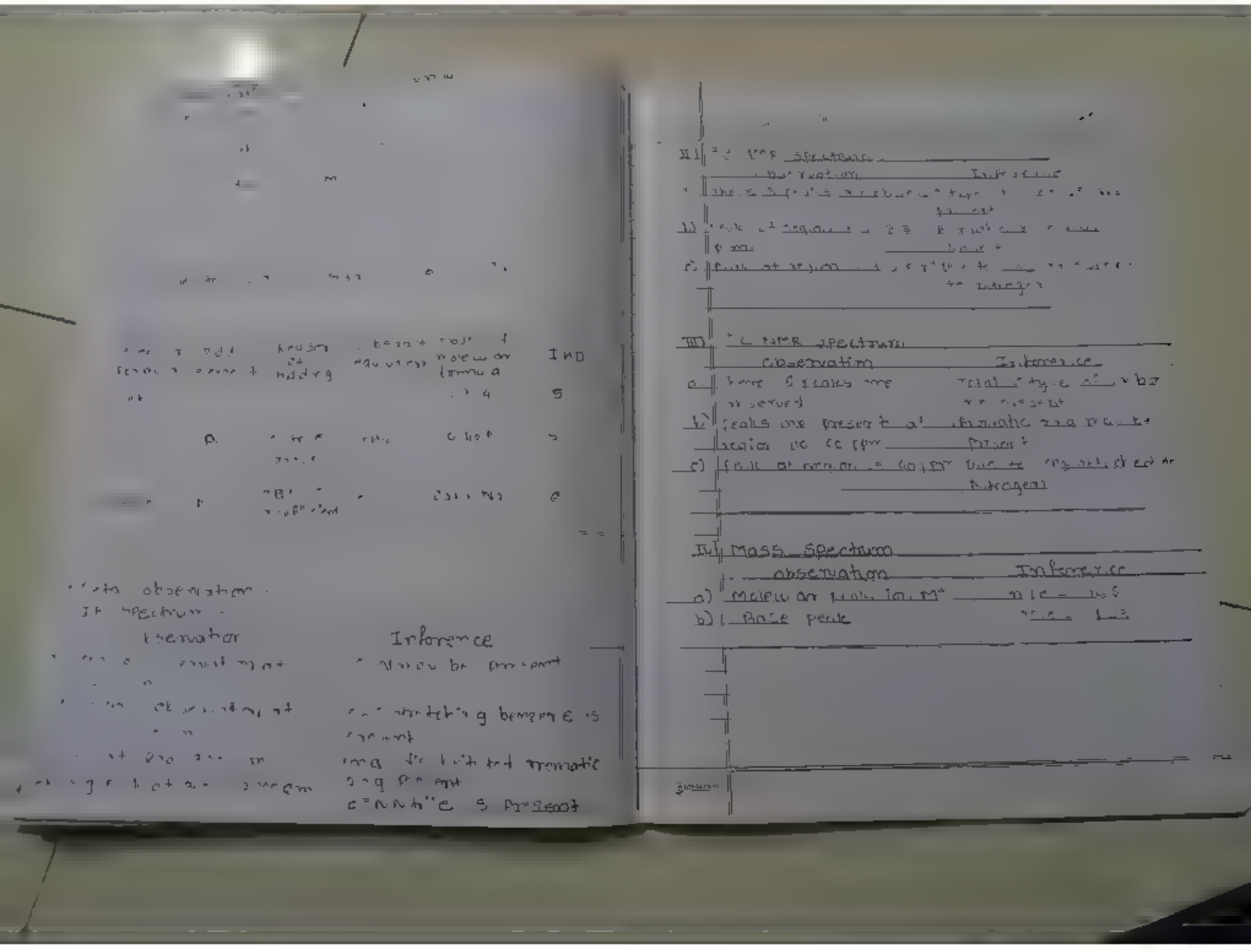
observation	Inference
a) Three type peaks observed	Total 3 types of hydrogen present
b) peak at δ = 7.5	Aromatic ring present

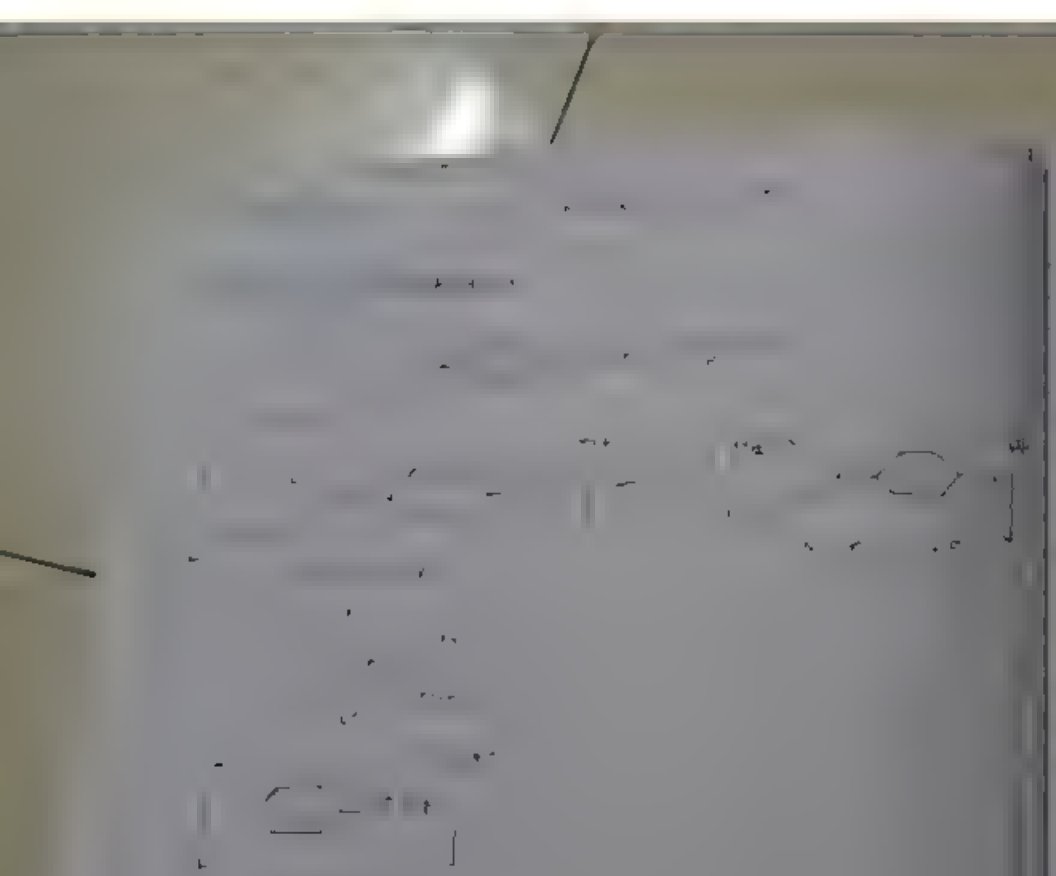
III. ^{13}C NMR Spectroscopy -

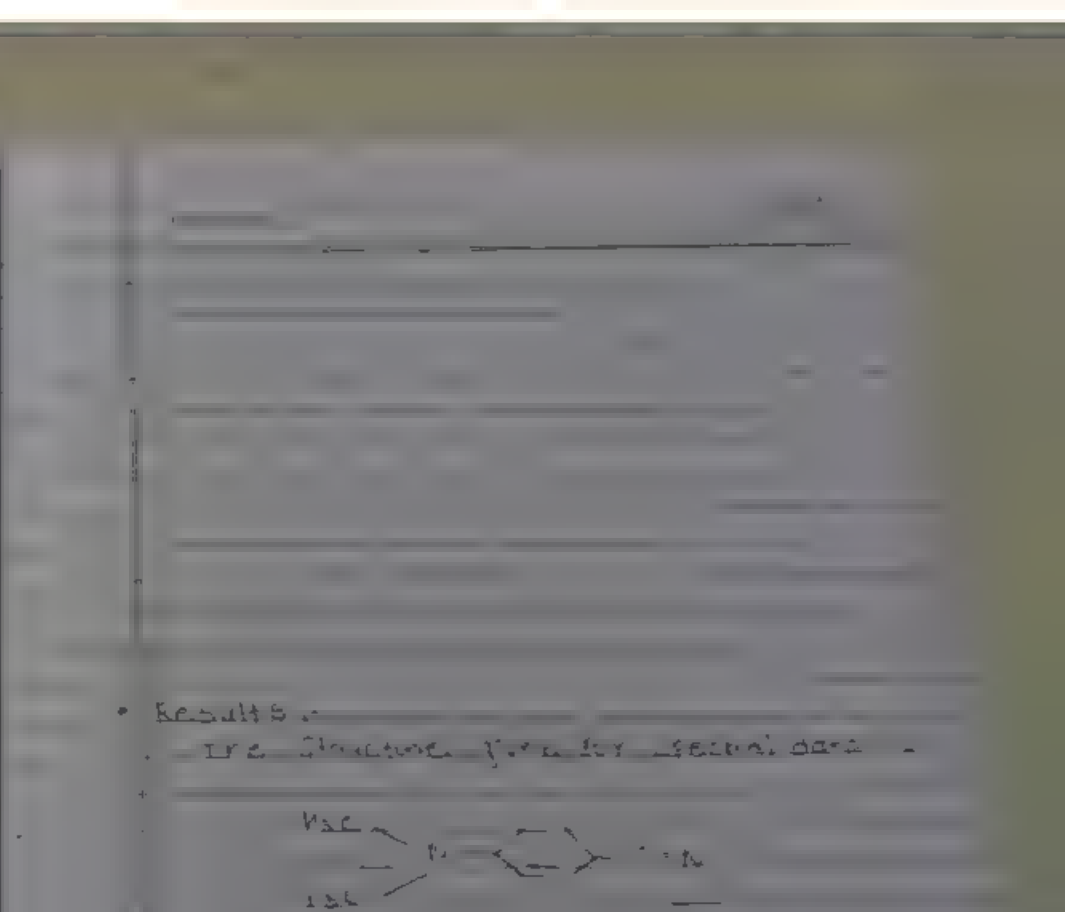
observation	Inference
a) There 6 peaks are observed	Total 6 type of carbons are present.
b) peak at region 110-160 ppm.	Aromatic ring may be present.

II. Mass Spectrum -

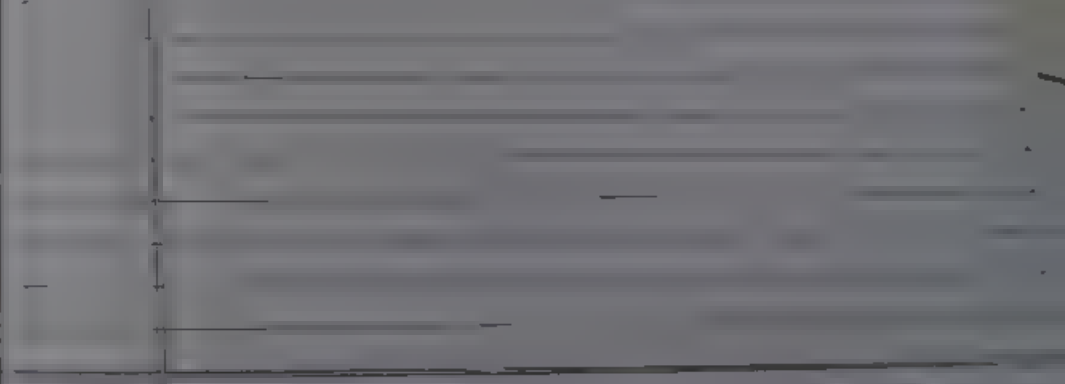
observation	Inference
a) Molecular peak ion m+	m/e = 146
b) Base peak	m/e = 145







- Results :



EXPERIMENT: No 10

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Date:

• Spectral identification NO - 10

A] preliminary observation -

I] IR spectroscopy

	observation	Inference
a)	strong observation at 3000 cm^{-1}	C-H stretching alkane may be present
b)	medium observation at 1500 - 1500 cm^{-1}	C=C stretching benzene may be present

II] ^{1}H NMR Spectroscopy -

	observation	Inference
a)	Two peaks are observed	Two type of protons are present.
b)	peak at 6-8 ppm.	Aromatic ring may be present.

III] ^{13}C NMR Spectroscopy -

	observation	Inference
a)	4 peaks are observed.	4 types of carbon are present.
b)	peak at 110 - 160 ppm.	Aromatic ring may be present.

IV] UV Spectrum -

	observation	Inference
a)	peak are abaut 220 nm	compound may be conjugated.

Teacher's Sign.:

II) mass spectrum -

Observation	Inference
a) Molecular peak ion	m/e = 182
b) Base peak	m/e = 91

- determination of molecular formula -

Rule of 13 = $\frac{M}{13}$ = n+r

no. of carbon = $\frac{M}{13} = \frac{182}{13} = 14$

no. of hydrogen = M - (C×12)
= 182 - (14×12)
= 182 - 168
= 14

Base formula :- $C_{nHnr} = C_{calculate} = C_{14}H_{14}$

IHD =

- Detail observation -

I] IR spectrum -

Observation	Inference
a) strong observation at 3000 cm^{-1}	C-H stretching alkane is present.
b) medium observation at region 700 - 800 cm^{-1}	mono - Substituted C-H stretching aromatic ring present
c) peaks at region 1600 - 1500 cm^{-1}	C=C stretching aromatic ring present.

II] ^1H NMR Spectrum -

observation	Inference
a) 2 peaks are present	2 type of Hydrogen present.
b) peak at 7.5-7.8 ppm.	Due to - C=C aromatic ring
c) peaks at 7-8 ppm	Aromatic ring present

III] ^{13}C NMR Spectrum

observation	Inference
a) 6 peaks are present	6 type of carbon present
b) peak at region 110-160 ppm	Aromatic ring present
c) peak at 30-60 ppm.	Due to - CH3 group present

IV] UV Spectrum -

observation	Inference
a) peak at above 220 nm	compound is conjugated

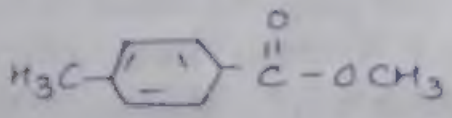
V] Mass Spectrum

Observation	Inference
a) Molecular peak ion M^+	m/e = 182
b) Base peak	m/e = 91

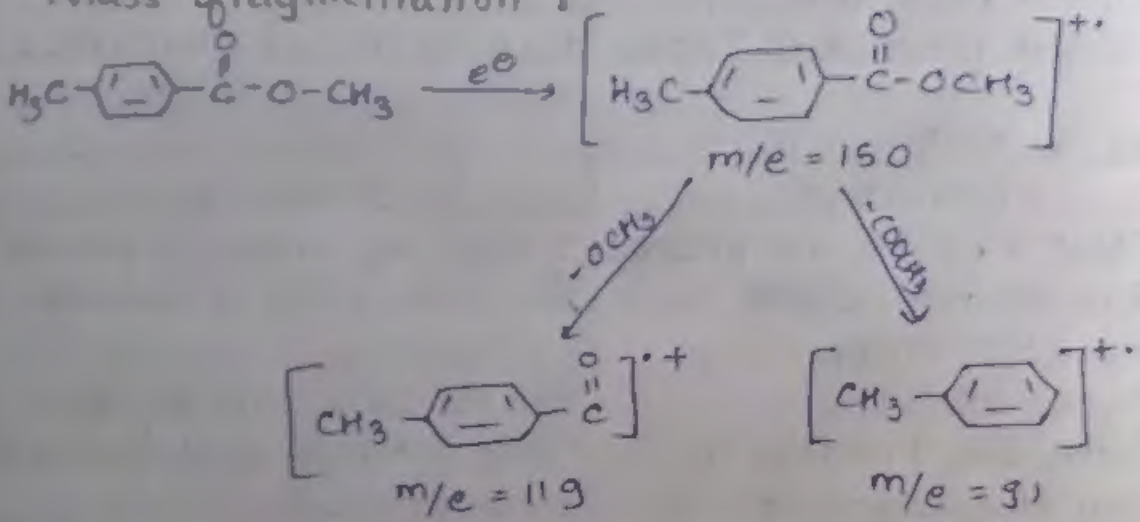
V] Mass Spectrum

Observation	Inference
a) Molecular ion peak $M^{+\cdot}$	m/e = 150
b) Base peak	m/e = 119

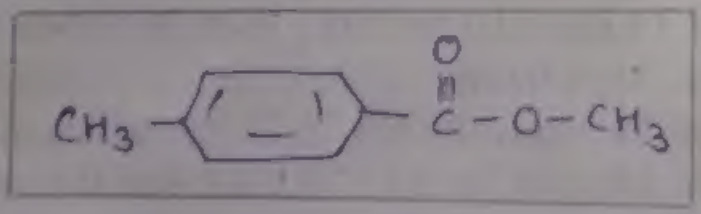
· Structure :



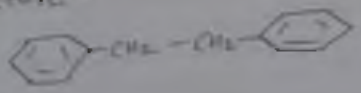
· Mass fragmentation :



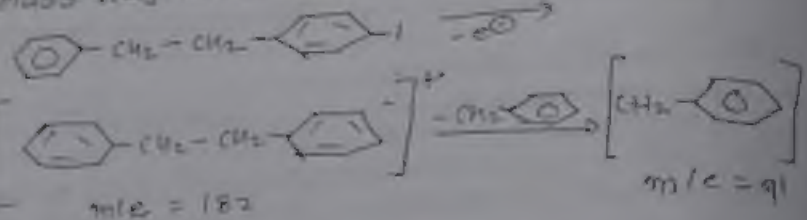
Thus, from above spectral evidence, the following structure can be confirmed.



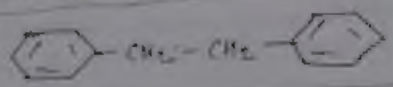
• structure -



• mass fragmentation -



The from spectral evidances the following structure is confirmed.



• Results -

The structure for given spectral data is